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14. ABSTRACT
The objective of this basic research effort is to provide the conceptual foundation for improved EM computational codes that can predict the propagation of EM waves through complex media (turbulent atmosphere and penetrable platforms) as well as wire antennas. The PI and his team will undertake the theoretical and numerical descriptions of well-conditioned numerical implementations (both surface integral equations and volumetric discretizations) of Maxwell's equations in various settings. These include open and closed surfaces (both smooth and rough), curved wires, and volumetric propagation with variations in the refractive index. The AF needs to have accurate and timely predictions of EM characteristics of various objects and media and the research pursued here will speak to those needs.

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Final Report

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Oscar P. Bruno

OBJECTIVES

* Volumetric propagation and scattering

* New Integral Equation Formulations and Solvers

* Offshoot methodologies

REPORT

The overall work in the proposed areas for the duration of this effort, through November 2010, is detailed in what follows. In particular, our efforts gave rise to 1) Volumetric propagation and scattering solvers for propagation through thousand of kilometers of realistic three-dimensional atmospheres (completed in 2009); 2) Development of high-order solvers, which do not suffer from restrictive CFL conditions, for solution of time-dependent wave-propagation problems in inhomogeneous media; 3) Electromagnetic integral solvers for open surfaces in three dimensions, with applicability to design of reflectarray antennas and negative-index materials; 4) Fast, high-order solvers for wire antenna problems; and 5) Solvers for general PDE problems which, not based on use of either finite elements or finite differences use the continuation method instead, and have been shown to lead to unconditionally stable numerics for a wide range of realistic PDE problems.

* VOLUMETRIC PROPAGATION AND SCATTERING

- PROPAGATION OF HIGH-FREQUENCY NONLINEAR WAVES THROUGH TISSUE:
  Our approach to this problem is based on the FC-AD algorithms

mentioned to some extent in the second subsection of the section "offshoot methodologies" below. Although the full Navier-Stokes equations for tissue can be adequately reduced to a second-order PDE for a single scalar unknown, recent numerical experiments (in a collaboration between Caltech's postdoctoral associate N. Albin and OB) have shown that, for a variety of reasons, the first-order system of Navier-Stokes equations is better suited for use in the present context. Indeed, first order systems do not require use of up-winding strategies (since, as we have shown, even without use of up-winding or other special treatments, the spectral FC-AD approach does not give rise to instabilities when used in connection with the first-order system). Further, the use of the Navier-Stokes equations retains all the nonlinear terms which for the high amplitudes in the focal region of a HIFU source have the potential to be non-negligible. Work in this area over the last year has lead to a highly efficient parallel solver capable of evaluating linear and nonlinear wave fields, as well as a solver for propagation in media with variable index of refraction.

- ATMOSPHERIC PROPAGATION: As part of this effort we developed a solver capable to evaluate propagation of waves across thousand of kilometers of realistic three-dimensional atmospheres: the best previous solvers were restricted to two-dimensional (range and height) refractive index variations. The numerical method we introduced in this context is applicable to non-spherically-symmetric atmospheric refractive index distributions that amount to sufficiently small perturbations from spherically symmetric smooth distributions; as shown through a variety of examples drawn from actual atmospheric data, the departures from spherical symmetry that actually occur in the Earth's atmosphere fall within the domain of applicability of the proposed methodology. One of the main elements of our algorithm is the well known Rytov approximation: we express a given atmospheric refractive index distribution n(r) as a sum n0(r) + n1(r) of an "unperturbed" spherically symmetric and smooth refractive index n0(r) and a small "perturbation" n1(r) which contains the three-dimensional variations of n(r). The character of the problem under consideration, however, is such that even its solution on the basis of Rytov's method gives rise to extremely high computational costs. We thus resort to (and extend) a high-frequency localization methodology introduced recently [Bruno, Geuzaine, Monro and Reitich, (2004), Bruno and Geuzaine, (2006)], which reduces computational costs in the high frequency regime through localization around the sets of points of stationary phase (which, as shown in our paper with J. Chaubell and C. Ao), actually coincide with light rays. In conjunction with this strategy, we evaluate the necessary spherically-symmetric Green's function by means of geometrical optics—which is permissible in view of our assumption of smoothness of the underlying unperturbed atmosphere. The solutions of the geometrical optics problems arising from both localization and evaluation of the spherically-symmetric Green's function are produced through high-order evaluation of integrals and differential operators, and, in particular, do not require use of numerical ODE solvers. Interestingly, unlike all other numerical methods applicable to this problem, the accuracy and computational costs of the proposed approach do not change as frequencies are increased. Thus, the proposed methodology will become even more attractive as it is applied to expected higher frequency (microwave) applications [Kursinski et al., (2002), Gorbunov, (2007)]. The validity of the Rytov approximation itself as a solver for problems of wave propagation within the atmosphere has been the subject of several discussions ([Brown, (1966), Brown (1967), Fried, (1967), Keller, (1969)]); roughly speaking, an application of the theory of [Brown, (1966)] indicates an agreement with our contention of validity for a tropospheric region of the order of 1000 km in horizontal dimensions. While Brown's theory ([Brown, (1966)]) is based on statistical assumptions that may be difficult to verify, the results presented in our work show unequivocally that under the types of refractive index variations present in the upper atmosphere, the Rytov approximation produces very accurate solutions for domains of thousands of kilometers in range.

* NEW INTEGRAL EQUATION FORMULATIONS AND SOLVERS

- NEW INTEGRAL EQUATIONS FOR OPEN SURFACES. As one of the central parts of the present effort we are developing a novel approach for the solution of problems of diffraction by open surfaces in three dimensional space. This methodology relies on use of weighted versions of the classical first-kind integral operators for the open-surface electromagnetic scattering problems (for which the unknowns do not tend to infinity), together with a generalization to the open-surface case of the well known closed-surface Calderon formulae. We had previously established for the acoustic case that, when used in conjunction with a spectrally accurate formulation and Krylov-subspace linear algebra solvers such as GMRES, the Calderon-like formulation produces results of high accuracy in very small numbers of iterations for both the Dirichlet and Neumann problems, and for low and high frequencies alike.

- SOLVERS APPLICABLE TO HIGHLY CHALLENGING GRATING DIFFRACTION PROBLEMS. In collaboration with M. Haslam we introduced a new algorithm for evaluation of electromagnetic and acoustic scattering by one-dimensional, perfectly conducting smooth periodic surfaces $z = f(x)$. Our algorithm is applicable to both TE and TM polarizations; in either case the problem is formulated in terms of a second-kind singular integral equation. Our high-order algorithm for these problems is based on two main elements: (i) Expansion of the unknown integral density in a Floquet series, and, (ii) Super- algebraically accurate treatment of integrals involving singular kernels. For an incident field with C1 smoothness, our algorithms converge faster than any integer power of M and N, where N denotes the number of surface-density unknowns, and M denotes the number of weights used for integration of the kernel functions. Progress in this area over the last year has given rise to solvers for non-graph diffractive surfaces _containing geometric singularities such as corners and edges_. The latter work resulted in the WCRM publication listed below.

- CURVED WIRE ANTENNAS SOLVERS. We developed an extension of the methodology previously put forward for straight wire antennas that applies to arbitrary curved wire antennas. We developed a general solver for open-ended general curved wire antennas, and we demonstrated the ability of our solvers to evaluate, with high accuracy, scattering by curved-wire problems hundreds of wavelengths in size in computing times of the order of minutes. Further, we demonstrated a capability to solve problems of radiation by antennas composed of large number of antenna elements.

- PARALLELIZATION OF SOLVERS FOR ACOUSTIC AND ELECTROMAGNETIC SCATTERING. Highly efficient algorithms were produced which can solve problems of scattering in parallel clusters. For example, our solvers demonstrated the largest direct solution ever obtained of a problems of scattering - containing a scatterer of a diameter of 400 wavelengths, and with an accuracy of four digits, in a 13 hour of computation in 256 processors at 2.7 GHz.

* OFFSHOOT METHODOLOGIES

- CONTINUATION-BASED "ALTERNATING DIRECTION" SOLVERS FOR GENERAL PDEs: FC-AD ALGORITHMS. A new methodology was introduced for the numerical solution of Partial Differential Equations in general spatial domains. The methodology is based on the use of the well-known Alternating Direction Implicit (ADI) approach of Peaceman and Rachford in conjunction with one-dimensional and high-order accurate Fourier representations of non-periodic data, obtained by way of the "continuation method" we introduced recently in the context of the problem of surface representation. These methodologies were further extended to enable treatment of problems involving Neumann boundary conditions, variable refractive indexes, and a parallel code was produced on the basis of a new method for "overlapping domain decomposition".

- CONTINUATION-BASED "EXPLICIT" SOLVERS FOR GENERAL PDEs and HYBRIDS: A variety of methods for solution of Partial Differential Equations on the basis of the Fourier Continuation method were developed, and are the subject of significant efforts at this time. Such solvers were applied to a variety of problems and configurations, including the Maxwell system, propagation of elastic waves in solids, convection diffussion problems in tissue, etc.

- COMPUTATIONAL BOUNDARY CONDITIONS. Many approaches have been proposed for this fundamental problem in the field of wave scattering. All of them fall into one of three main categories. The first class of methods is based on mathematical approximations or physical heuristics. These boundary conditions are often local in space and time, therefore easy to implement and run in short computing times. However, these approaches give rise to spurious refleections at the artificial boundary, no matter how refined the discretization is, which travel back into the computational domain and corrupt the solution. A second group consists of accurate and convergent methods. However, these formulations are usually nonlocal in time and space, thus harder to implement and often more expensive than the computation of the interior scheme itself. Finally, there are methods which are accurate and fast. These approaches are often local in time, and the nonlocality in space is confined to a closed surface rather than the whole computational domain. The drawback of these approaches lies in the fact that the outer boundary must be taken to be either a sphere, a plane, or a cylinder. For many applications of interest, this may require use of a computational domain much larger than actually needed, which leads to an expensive overall numerical scheme. In our work for this problem we introduced a new methodology in order to compute the fields at the artificial boundary. The boundary condition is both nonlocal in space and time, but the nonlocal behavior is confined to a finite number of points in time and to a surface in space. Like the second class of methods described above, the proposed algorithm is accurate and numerically convergent, yet its computational cost is less than the underlying portion of the volumetric calculation. And, unlike the third category, this new approach allows us to choose the artificial boundary to be arbitrarily close to the scatterer. This method is based on a concept of "sparse equivalent sources" representations (introduced by the PI in collaboration with L. Kunyansky) which allows a highly accurate and fast evaluation of the boundary condition when used in combination with fast Fourier transforms. A variety of numerical results we produced for three dimensional problems demonstrate the accuracy, high-order ocnvergence and effectiveness of the methodology.

RELEVANT PUBLICATIONS

"Mathematical analysis of a fast, high order Nystrom method for BIEs solution of three-dimensional scattering problems", O. Bruno, V. Dominguez and F. Sayas, Preprint, 2011

"A highly accurate integral method for open-surface scattering requiring small numbers of GMRES iterations", O. Bruno and Stephane Lintner, In preparation.

"Well-posed Integral Equations for Acoustic Problems on Open
Surfaces", O. Bruno and Stephane Lintner, In preparation.

"Well-conditioned high-order algorithms for the solution of
three-dimensional surface acoustic scattering problems with Neumann
boundary conditions", Bruno O., T. Elling, C. Turc, preprint (2010)

"Numerical simulation of focused nonlinear acoustic beams: a new
FC-based direct solver and comparisons to the KZK approximation",
Nathan Albin, Oscar P. Bruno, Theresa Y. Cheung and Robin
O. Cleveland, preprint, (2011)

"A Spectral FC Solver for the Compressible Navier-Stokes Equations in
General Domains I: Explicit time-stepping" Nathan Albin and Oscar
P. Bruno, To appear in Journal of Computational Physics (2011)

"Efficient high-order evaluation of scattering by periodic surfaces:
vector-parametric gratings and geometric singularities", O. P. Bruno
and M. Haslam, Waves in Complex and Random Media, Vol 20, 1745--5049
(2010)

"High-order unconditionally-stable FC-AD solvers for general smooth
domains I. Basic elements", O. Bruno and M. Lyon, Journal of
Computational Physics, 2009–-2033 (2010).

"High-order unconditionally-stable FC-AD solvers for general smooth
domains II. Elliptic, Parabolic and Hyperbolic PDEs; Theoretical
considerations", Journal of Computational Physics 229, 3358--3381
(2010)

"Efficient high-order evaluation of scattering by periodic surfaces:
deep gratings, high frequencies and glancing incidences", O. P. Bruno
and M. Haslam; Journal of the Acoustical Society of America, 658-668
(2009)

"Electromagnetic integral equations requiring small numbers of
Krylov-subspace iterations", Bruno O., T. Elling, R. Paffenroth,
C. Turc, Journal of Computational Physics, 6169–6183 (2009)

Bruno O., J. Ovall, C. Turc, “A high-order integral algorithms for
highly singular PDE solutions in Lipschitz domains”, Computing 84,
149–181 (2009)

"Evaluation of EM-wave propagation in fully three-dimensional
atmospheric refractive index distributions", J. Chaubell, O. P. Bruno
and C. O. Ao, Radio Science, Vol. 44, RS1012,
doi:10.1029/2008RS003882, (2009).

INDUSTRIAL CONTACTS AND COLLABORATIONS

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Dr. Martin Pietraszkiewicz, Northrop Grumman Space Technology

HONORS/AWARDS (2007-2011)

Keynote lecture at the 24th Biennial Numerical Analysis conference, University of Strathclyde, Glasgow, June 28th- July 1st 2011.

Plenary speaker at "Frontiers in Applied and Computational Mathematics" (FACM) to be held at the New Jersey Institute of Technology, June 9-11, 2011

Plenary speaker at the Isaac Newton Institute: conference on highly oscillatory problems, 12--17 September 2010.

Plenary Speaker, ICOSAHOM 2009, Norwegian University of Science and Technology in Trondheim, Norway, July 22-26, 2009

Plenary Speaker at the Oberwolfach meeting on "Analysis of boundary element methods"; Martin Costabel and Ernst P. Stephan, Organizers, April 13th - 19th, 2008.

Plenary Speaker, Workshop on wave scattering problems, France , December 12-14, 2007

Organizer of the workshop "High-order methods for computational wave propagation and scattering" (w. R. Kress) at the American Institute of Mathematics, Palo Alto, CA, 2007.

Plenary Speaker, Leading lecture, at the Isaac Newton Institute Workshop Effective Computational Methods for Highly Oscillatory Problems: The Interplay between Mathematical Theory and Applications 2 July to 6 July 2007; Isaac Newton Institute, Cambridge CB3 0EH,

Plenary Speaker: Workshop on Oscillatory integrals and integral equations in high frequency scattering and wave propagation", June 19, 2007. A one-day workshop at the Isaac Newton Institute 20 Clarkson Road, Cambridge CB3 0EH, UK.

Plenary Speaker at the Oberwolfach meeting on Computational Electromagnetism and Acoustics, February 5 to 9th, 2007.

Plenary Speaker at the Seventh Mississippi State - UAB Conference on Differential Equations \& Computational Simulations November 1-3, 2007

Doubletree Hotel Birmingham, AL, USA.